Supplemental information

The molecular architecture of the nuclear basket

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The Molecular Architecture of the Nuclear Basket

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Table S1. Information and spatial restraints for Integrative modeling of yeast and mouse basket. **Related to Figures 3-5 and Figures S4-S6.**
For each basket model (column 1), a list of experimental techniques is shown in column 2 that provide the spatial information (column 3) for Integrative modeling. Column 4 provides a reference to the original dataset or method.

Model	Experimental Technique	Spatial Information	Reference
Yeast	Quantitative mass spectrometry and biochemical quantification	Stoichiometry of Nups (**Table S2**)	Kim et al., 2018[1]
	Chemical cross-linking with mass spectrometry readout	626 intra and intermolecular crosslinks among yNups and yMlps	Kim et al., 2018 and Niepel et al., 2013[1,2] & This paper
	Cryo-ET	The overall shape of the basket, including the basket distal density	This paper
	Integrative models and atomic structural models	yNup84 complex dimer model, yNup2 structural model (**Table S2**)	Akey et al., 2022, Jumper et al., 2021, Varadi et al. 2022[3–5]
	Bioinformatics information	Sequence information, coiled-coil propensities of the yMlps, alignments. Connectivity between residues.	McDonnell et al., 2006[6]
	Immuno-EM	Upper and lower bound on the N-/C- terminus of yMlps	Niepel et al., 2013[2]
	Biochemical experiments including *in vitro* binding assays, proximity labeling	Interactions between yNup60[MBM] (240-318) and yMlp1 (382-620), Interaction between yNup60[N2BM] (505-539) and yNup2 (83-136), nuclear envelope binding domain of yNup1, yNup60	Cibulka et al. 2022, and Meszaros et al. 2015[7,8]
Mouse/Human	Quantitative mass spectrometry and biochemical quantification	Stoichiometry of Nups (**Table S3**)	Li et al., 2021 and Ori et al., 2013[9,10]
	Cryo-ET	The overall shape of the basket, including the basket distal density	This study
	Integrative models and atomic structural models	mNup107 complex dimer model, mNup50 structural model (**Table S3**)	Jumper et al., 2021, Mosalaganti et al., 2022, Sali et al., 1993, Varadi et al., 2022 and

			Eeswat et al., 2007[4,5,11–13]
	Bioinformatics information	Sequence information, coiled-coil propensities of the mTprs, orthologs alignments. Connectivity between residues/beads. Structural equivalent distances between ortholog Nups.	McDonnell et al., 2006[6]
	Immuno-EM	Upper and lower bound on the N-/C- terminus of mTprs	Frosst et al.,2002[14]
	Biochemical experiments including proximity labeling	Nuclear envelope binding domains of mNup153	Vollmer et al., 2015[15]

Table S2. Summary of the Integrative modeling of the yBasket. Related to Figures 3-5 and Figures S4-S6.

1) Gathering data	
Prior models	yNup84 complex dimer (PDB id: 7n84)[3] Position of yNup84 complex derived by fitting on cryo-ET map using the chimera *fit map* feature[16,17]. yNup2 alphaFold model (AF-P32499-F1-model_v4.pdb) [4,5,18] Generic Mlps coiled-coil segments models[19]
Physical principles and statistical preferences	Excluded volume Sequence connectivity
Experimental information	**See Table S1**
2) Representing the system	
Sequences (Uniprot Ids)	yMlp1:Q02455, yMlp2:P40457, yMlp:Poly-ala of length yMlp1, yNup1:P20676, yNup2:P32499, yNup60:P39705, yNup120:P35729, yNup85:P46673, yNup145c:P49687, ySec13:Q04491, ySeh1:P53011, yNup84:P52891, yNup133:P36161
Composition (number of copies)	yMlp:2, yNup1:1, yNup2:2, yNup60:2, yNup120:2, yNup85:3, yNup145c:2, ySec13:2, ySeh1:2, yNup84:2, yNup133:2
Atomic (structured) components	yMlp.0: 71-183, 197-221, 239-281, 285-324, 340-371, 435-463, 535-570, 575-617, 622-668, 689-717, 745-773, 791-840, 844-893, 930-986, 990-1088, 1092-1127, 1143-1199, 1212-1251, 1254-1286, 1290-1339, 1343-1385, 1408-1457, yMlp.1: 71-183, 197-221, 239-281, 285-324, 340-371, 435-463, 535-570, 575-617, 622-668, 689-717, 745-773, 791-840, 844-893, 930-986, 990-1088, 1092-1127, 1143-1199, 1212-1251, 1254-1286, 1290-1339, 1343-1385, 1408-1457, yNup1.0: 1-32, 85-104, 106-123, yNup2.0: 83-136, 602-720, yNup2.1: 83-136, 602-720, yNup60.0: 27-47, 91-104, 106-119, 121-140, 142-162, yNup60.1: 27-47, 91-104, 106-119, 121-140, 142-162, yNup120.0: 1-29, 53-305, 311-711, 714-1036, yNup120.1: 1-29, 53-305, 311-711, 714-1036, yNup133.0: 63-183, 198-480, 490-763, 772-1155, yNup133.1: 56-77, 86-125, 133-144, 162-184, 193-200, 206-249, 258-480, 490-763, 772-1155, yNup145c.0: 119-712, yNup145c.1: 119-712, yNup84.0: 7-20, 27-80, 96-126, 136-364, 372-483, 506-562, 575-726, yNup84.1: 7-20, 27-80, 96-126, 136-364, 372-483, 506-562, 575-726, yNup85.0: 47-126, 132-230, 235-436, 451-744, yNup85.1: 47-126, 132-230, 235-436, 451-739, yNup85.2: 47-126, 132-230, 235-436, 451-739, ySec13.0: 8-157, 170-293, ySec13.1: 8-157, 170-293, ySeh1.0: 1-248, 288-346, ySeh1.1: 1-248, 288-346

Unstructured components	yMlp.0:-NTD: 1-70, yMlp.1:-NTD 1-70, yMlp.0:-LOOP: 184-196, 222-238, 282-284, 325-339, 372-434, 464-534, 571-574, 618-621, 669-688, 718-744, 774-790, 841-843, 894-929, 987-989, 1089-1091, 1128-1142, 1200-1211, 1252-1253, 1287-1289, 1340-1342, 1386-1407, yMlp.1:-LOOP: 184-196, 222-238, 282-284, 325-339, 372-434, 464-534, 571-574, 618-621, 669-688, 718-744, 774-790, 841-843, 894-929, 987-989, 1089-1091, 1128-1142, 1200-1211, 1252-1253, 1287-1289, 1340-1342, 1386-1407, yMlp.0:-CTD: 1458-1875, yMlp.1:-CTD: 1458-1875, yNup1.0: 33-84, 105-105, 124-335, yNup2.0: 51-82, yNup2.1: 51-82, yNup60.0: 1-26, 48-90, 105-105, 120-120, 141-141, 163-398, 505-539, yNup60.1: 1-26, 48-90, 105-105, 120-120, 141-141, 163-398, 505-539, yNup120.0: 30-52, 306-310, 712-713, 1037-103, yNup120.1: 30-52, 306-310, 712-713, 1037-1037, yNup133.0: 1-62, 184-197, 481-489, 764-771, 1156-1157, yNup133.1: 1-55, 78-85, 126-132, 145-161, 185-192, 201-205, 250-257, 481-489, 764-771, 1156-115, yNup145c.0: 1-118, yNup145c.1: 1-118, yNup84.0: 1-6, 21-26, 81-95, 127-135, 365-371, 484-505, 563-574, yNup84.1: 1-6, 21-26, 81-95, 127-135, 365-371, 484-505, 563-574, yNup85.0: 1-46, 127-131, 231-234, 437-450, yNup85.1: 1-46, 127-131, 231-234, 437-450, 740-744, yNup85.2: 1-46, 127-131, 231-234, 437-450, 740-744, ySec13.0: 1-7, 158-169, 294-297, ySec13.1: 1-7, 158-169, 294-297, ySeh1.0: 249-287, 347-349, ySeh1.1: 249-287, 347-349
Resolutions of structured components	1 [R1] residue per bead and 30 [R30] residue per bea
Resolutions of unstructured components	yMlp.0-NTD: 50 [R50] residue per bead yMlp.1-NTD: 50 [R50] residue per bead yMlp.0-LOOP: 5 [R5] residue per bead yMlp.1-LOOP: 5 [R5] residue per bead yMlp.0-CTD: 50 [R50] residue per bead yMlp.1-CTD: 50 [R50] residue per bead Rest all unstructured components 30 [R30] residue per bead
Structural coverage	77.39%
Rigid body (RB) definitions	RB1: yMlp.0 71-183, yMlp.1 71-183, RB2: yMlp.0 197-221, yMlp.1 197-221, RB3: yMlp.0 239-281, yMlp.1 239-281, RB4: yMlp.0 285-324, yMlp.1 285-324, RB5: yMlp.0 340-371, yMlp.1 340-371, RB6: yMlp.0 435-463, yMlp.1 435-463, RB7: yMlp.0 535-570, yMlp.1 535-570, RB8: yMlp.0 575-617, yMlp.1 575-617, RB9: yMlp.0 622-668, yMlp.1 622-668, RB10: yMlp.0 689-717, yMlp.1 689-717, RB11: yMlp.0 745-773, yMlp.1 745-773, RB12: yMlp.0 791-840, yMlp.1 791-840, RB13: yMlp.0 844-893, yMlp.1 844-893, RB14: yMlp.0 930-986, yMlp.1 930-986, RB15: yMlp.0 990-1088, yMlp.1 990-1088, RB16: yMlp.0 1092-1127, yMlp.1 1092-1127, RB17: yMlp.0 1143-1199, yMlp.1 1143-1199, RB18: yMlp.0 1212-1251, yMlp.1 1212-1251, RB19: yMlp.0 1254-1286, yMlp.1 1254-1286, RB20: yMlp.0 1290-1339, yMlp.1 1290-1339, RB21: yMlp.0 1343-1385, yMlp.1 1343-1385, RB22: yMlp.0 1408-1457, yMlp.1 1408-1457, RB23: yNup1.0 1-32, RB24: yNup1.0 85-104, RB25: yNup1.0 106-123, RB26: yNup2.0 83-136, RB27: yNup2.0 602-720, RB28: yNup2.1 83-136, RB29: yNup2.1 602-720, RB30: yNup60.0 27-47, RB31: yNup60.0 91-104, RB32: yNup60.0 106-119, RB33: yNup60.0 121-140, RB34: yNup60.0 142-162, RB35: yNup60.1 27-47, RB36: yNup60.1 91-104, RB37: yNup60.1 106-119, RB38: yNup60.1 121-140, RB39: yNup60.1 142-162, RB40: yNup120.0 1-29, yNup120.0 53-305, yNup120.0 311-711, yNup120.0 714-1036, RB41: yNup120.1 1-29, yNup120.1 53-305, yNup120.1 311-711, yNup120.1 714-1036, RB42: yNup85.0 47-126, yNup85.0 132-230, yNup85.0 235-436, yNup85.0 451-744, RB43: yNup85.1 47-126, yNup85.1 132-230, yNup85.1 235-436, yNup85.1 451-739, RB44: yNup85.2 47-126, yNup85.2 132-230, yNup85.2 235-436, yNup85.2 451-739, RB45: yNup145c.0 119-712, RB46: yNup145c.1 119-712, RB47: ySec13.0 8-157, ySec13.0 170-293, RB48: ySec13.1 8-157, ySec13.1 170-293, RB49: ySeh1.0 1-248, ySeh1.0 288-346, RB50: ySeh1.1 1-248, ySeh1.1 288-346, RB51: yNup84.0 7-20, yNup84.0 27-80, yNup84.0

	96-126, yNup84.0 136-364, yNup84.0 372-483, yNup84.0 506-562, yNup84.0 575-726, RB52:yNup84.1 7-20, yNup84.1 27-80, yNup84.1 96-126, yNup84.1 136-364, yNup84.1 372-483, yNup84.1 506-562, yNup84.1 575-726, RB53: yNup133.0 63-183, yNup133.0 198-480, yNup133.0 490-763, yNup133.0 772-1155, RB54: yNup133.1 56-77, yNup133.1 86-125, yNup133.1 133-144, yNup133.1 162-184, yNup133.1 193-200, yNup133.1 206-249, yNup133.1 258-480, yNup133.1 490-763, yNup133.1 772-1155
Spatial restraints encoded into scoring functions	Excluded volume; applied to the R30 representation Sequence connectivity; applied to the R1 representation Cross-link restraints; applied to the R1 representation

3) Structural sampling

Sampling method	Replica Exchange Gibbs sampling, based on Metropolis Monte Carlo[20,21]
Replica exchange temperature range	1.0 - 4.0
Number of replicas	4
Number of Independent runs	300
Number of structures generated	15,467,933
Movers for flexible string of beads	Random translation up to 10 Å
Total time for sampling	180 hours on 1200 processors

4) Validating the yBasket models

Models selected for validation	
Equilibrated models	2,335,171
Number of structures in samples A/B	All: 1,210,882 / 1,072,745
Number of structures selected for RMSD clustering sample A/B	Random sub-sample: 7,857 / 7,987
p-value of non-parametric Kolmogorov-Smirnov two-sample test	0.0556 (threshold p-value > 0.05)
Kolmogorov-Smirnov two-sample test statistic, D	0.0
Throughness of the structural sampling	
Sampling precision	70.41 Å
Homogeneity of proportions χ^2-test (p-value)/Cramers V value	0.0/0.095 (thresholds: p-value<0.05 OR Cramer's V<0.1)
Number of clusters	5
Cluster populations	Cluster 1 : 93.5%, Cluster 2 : 4.0%, Cluster 3 : 1.2%, Cluster 4 : 1.0%, Cluster 5 : 0.3%
Cluster precisions	Cluster 1 : 57.2 Å, Cluster 2 : 58.6 Å, Cluster 3 : 56.5 Å, Cluster 4 : 53.3 Å, Cluster 5 : 59.8 Å

Average cross-correlation between localization probability densities of samples A and B	0.96
Validation by information used for modeling	
Percent of sequence connectivity restraints satisfied by ensemble	99%
Percent Excluded volume restraint satisfied by ensemble	Mean value 99.2% at R[30] resolution and mean value 99.9% at R[1] resolution
Cross-correlation between localization probability densities and cryo-ET map	0.82
Percent crosslink restraint satisfied by ensemble	94%
5) Software and data availability	
Software	
Modeling programs	IMP PMI module, version-a41075a Integrative Modeling Platform (IMP), version 2.19 (https://integrativemodeling.org)[22] gmconvert[23]
Modeling scripts	https://github.com/neeleshsoni21/Yeast_NPC_Basket
Structure prediction	AlphaFold2
Visualization and plotting	UCSF Chimerax
Data	
PDB-dev accession code	Collection of all models (PDBDEV: PDBDEV_G_1000004) and Yeast NPC (PDBDEV: PDBDEV_00000386, DBDEV: PDBDEV_00000387).

Table S3. Summary of the Integrative modeling of the mBasket. Related to Figures 3-5 and Figures S4-S6.

1) Gathering data	
Prior models	mNup107 complex dimer comparative model built on Human Nup107 complex (PDB id: 7r5j)[11–13] Position of yNup107 complex derived by fitting on cryo-ET map using the chimera *fit map* feature[16,17]. yNup50 alphaFold model (AF-Q9JIH2-F1-model_v4.pdb) [4,5,18] Tpr coiled-coil segments models[19]
Physical principles and statistical preferences	Excluded volume Sequence connectivity
Experimental information	**See Table S1**
2) Representing the system	
Sequences (Uniprot Ids)	mTpr:F6ZDS4, mNup50:Q9JIH2, mNup153:E9Q3G8,

	mNup43:P59235, mSeh1:Q8R2U0, mNup98-mNup96:Q6PFD9, mNup85:Q8R480, mNup37:Q9CWU9, mNup107:Q8BH74, mSec13:Q9D1M0, mNup133:Q8R0G9, mNup160:Q9Z0W3
Composition (number of copies)	mTpr: 2, mNup50: 2, mNup153: 2, mNup107: 2, mNup133: 2, mNup160: 2, mNup37: 2, mNup43: 2, mNup85: 2, mNup96: 2, mSec13: 2, mSeh1: 2
Atomic (structured) components	mTpr.0: 96-120, 124-180, 187-247, 254-285, 289-356, 360-405, 413-451, 511-595, 639-681, 757-883, 901-946, 947-999, 1004-1060, 1064-1106, 1107-1131, 1135-1163 1170-1201, 1205-1254, 1281-1337, 1343-1420, 1424-1491, 1543-1616, 1627-1690, mTpr.1: 96-120, 124-180, 187-247, 254-285, 289-356, 360-405, 413-451, 511-595, 639-681, 757-883, 901-946, 947-999, 1004-1060, 1064-1106, 1107-1131, 1135-1163, 1170-1201, 1205-1254, 1281-1337, 1343-1420, 1424-1491, 1543-1616, 1627-1690, mNup50.0: 151-204, 355-466, mNup50.1: 151-204, 355-466, mNup153.0: 36-57, mNup153.1: 36-57, mNup107.0: 145-926, mNup107.1: 145-926, mNup133.0: 70-1155, mNup133.1: 70-1155, mNup160.0: 1-1402, mNup160.1: 1-1402, mNup37.0: 1-326, mNup37.1: 1-326, mNup43.0: 1-292, 327-380, mNup43.1: 1-292, 327-380, mNup85.0: 1-656, mNup85.1: 1-656, mNup96.0: 1111-1159, 1194-1816, mNup96.1: 1111-1159, 1194-1816, mSec13.0: 1-302, mSec13.1: 1-302, mSeh1.0: 1-324, mSeh1.1: 1-324
Unstructured components	mTpr.0:-NTD: 1-95, mTpr.1:-NTD: 1-95, mTpr.0:-LOOP: 121-123, 181-186, 248-253, 286-288, 357-359, 406-412, 452-510, 596-638, 682-756, 884-900, 1000-1003, 1061-1063, 1132-1134, 1164-1169, 1202-1204, 1255-1280, 1338-1342, 1421-1423, 1492-1542, 1617-1626, mTpr.1:-LOOP: 1-95, 121-123, 181-186, 248-253, 286-288, 357-359, 406-412, 452-510, 596-638, 682-756, 884-900, 1000-1003, 1061-1063, 1132-1134, 1164-1169, 1202-1204, 1255-1280, 1338-1342, 1421-1423, 1492-1542, 1617-1626, mTpr.0:-CTD: 1691-2431, mTpr.1:-CTD: 1691-2431, mNup50.0: 1-150, 205-354, mNup50.1: 1-150, 205-354, mNup153.0: 1-35, 58-428, 540-574, mNup153.1: 1-35, 58-428, 540-574
Resolutions of structured components	1 [R1] residue per bead and 30 [R30] residue per bead
Resolutions of unstructured components	mTpr.0-NTD: 50 [R50] residue per bead mTpr.1-NTD: 50 [R50] residue per bead mTpr.0-LOOP: 30 [R5] residue per bead mTpr.1-LOOP: 30 [R5] residue per bead mTpr.0-CTD: 50 [R50] residue per bead mTpr.1-CTD: 50 [R50] residue per bead Rest all unstructured components 30 [R30] residue per bead
Structural coverage	79.48%
Rigid body (RB) definitions	RB1: mTpr.0 96-120, mTpr.1 96-120, RB2: mTpr.0 124-180, mTpr.1 124-180, RB3: mTpr.0 187-247, mTpr.1 187-247, RB4: mTpr.0 254-285, mTpr.1 254-285, RB5: mTpr.0 289-356, mTpr.1 289-356, RB6: mTpr.0 360-405, mTpr.1 360-405, RB7: mTpr.0 413-451, mTpr.1 413-451, RB8: mTpr.0 511-595, mTpr.1 511-595, RB9: mTpr.0 639-681, mTpr.1 639-681, RB10: mTpr.0 757-883, mTpr.1 757-883, RB11: mTpr.0 901-946, mTpr.1 901-946, RB12: mTpr.0 947-999, mTpr.1 947-999, RB13: mTpr.0 1004-1060, mTpr.1 1004-1060, RB14: mTpr.0 1064-1106, mTpr.1 1064-1106, RB15: mTpr.0 1107-1131, mTpr.1 1107-1131, RB16: mTpr.0 1135-1163, mTpr.1 1135-1163, RB17: mTpr.0 1170-1201, mTpr.1 1170-1201, RB18: mTpr.0 1205-1254, mTpr.1 1205-1254, RB19: mTpr.0 1281-1337, mTpr.1 1281-1337, RB20: mTpr.0 1343-1420, mTpr.1 1343-1420, RB21: mTpr.0 1424-1491, mTpr.1 1424-1491, RB22: mTpr.0 1543-1616, mTpr.1 1543-1616, RB23: mTpr.0 1627-1690, mTpr.1 1627-1690, RB24: mNup50.0 151-204, RB25: mNup50.0 355-466, RB26: mNup50.1 151-204, RB27: mNup50.1 355-466, RB28: mNup153.0

	36-57, RB29: mNup153.1 36-57
	Fixed RB components: RB30: mNup160.0 1-1402, RB31: mNup160.1 1-1402, RB32: mNup85.0 1-656, RB33: mNup85.1 1-656, RB34: mNup96.0 1111-1159, mNup96.0 1194-1816, RB35: mNup96.1 1111-1159, mNup96.1 1194-1816, RB36: mSec13.0 1-302, RB37: mSec13.1 1-302, RB38: mSeh1.0 1-324, RB39: mSeh1.1 1-324, RB40: mNup107.0 145-926, RB41: mNup107.1 145-926, RB42: mNup133.0 70-1155, RB43: mNup133.1 70-1155, RB44: mNup37.0 1-326, RB45: mNup37.1 1-326, RB46: mNup43.0 1-292, mNup43.0 327-380, RB47: mNup43.1 1-292, mNup43.1 327-380
Spatial restraints encoded into scoring functions	Excluded volume; applied to the R30 representation Sequence connectivity; applied to the R1 representation Cross-link restraints; applied to the R1 representation

3) Structural sampling

Sampling method	Replica Exchange Gibbs sampling, based on Metropolis Monte Carlo [20,21]
Replica exchange temperature range	1.0 - 4.0
Number of replicas	2
Number of Independent runs	200
Number of structures generated	9,569,309
Movers for flexible string of beads	Random translation up to 10 Å
Total time for sampling	168 hours on 400 processors

4) Validating the mBasket models

Models selected for validation	
Equilibrated models	1,216,228
Number of structures in samples A/B	All: 520,767 / 474,386
Number of structures selected for RMSD clustering sample A/B	Random sub-sample: 6,886 / 7,783
p-value of non-parametric Kolmogorov-Smirnov two-sample test	0.056 (threshold p-value > 0.05)
Kolmogorov-Smirnov two-sample test statistic, D	0.0

Throughness of the structural sampling	
Sampling precision	52.9 Å
Homogeneity of proportions χ^2-test (p-value)/Cramers V value	0.0/0.097 (thresholds: p-value<0.05 OR Cramer's V<0.1)
Number of clusters	4

Cluster populations	Cluster 1 : 75.6%, Cluster 2 : 15.6%, Cluster 3 : 8.1%, Cluster 4 : 0.7%
Cluster precisions	Cluster 1 : 41.9 Å, Cluster 2 : 34.9 Å, Cluster 3 : 41.2 Å, Cluster 4 : 31.4 Å
Average cross-correlation between localization probability densities of samples A and B	0.95
Validation by information used for modeling	
Percent of sequence connectivity restraints satisfied by ensemble	99%
Percent Excluded volume restraint satisfied by ensemble	Mean value 94.55% at R[30] resolution and mean value 99.63% at R[1] resolution
Cross-correlation between localization probability density and cryo-ET map	0.87
5) Software and data availability	
Software	
Modeling programs	IMP PMI module, version-a41075a Integrative Modeling Platform (IMP), version 2.19 (https://integrativemodeling.org) [22] Gmconvert [23]
Modeling scripts	https://github.com/neeleshsoni21/Mouse_NPC_Basket
Structure prediction	AlphaFold2
Visualization and plotting	UCSF Chimerax
Data	
PDB-dev accession code	Collection of all models (PDBDEV: PDBDEV_G_1000004) and Mammalian NPC (PDBDEV: PDBDEV_00000384, PDBDEV: PDBDEV_00000385)

References

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